State-specific hydrogenic recombination cooling coefficients for a wide range of conditions[1]

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Abstract

Recombination cooling, in which a free electron emits light while being captured to an ion, is an important cooling process in photoionized clouds that are optically thick or have low metallicity. State specific rather than total recombination cooling rates are needed since the hydrogen atom tends to become optically thick in high-density regimes such as Active Galactic Nuclei. This paper builds upon previous work to derive the cooling rate over the full temperature range where the process can be a significant contributor in a photoionized plasma. We exploit the fact that the recombination and cooling rates are given by intrinsically similar formulae to express the cooling rate in terms of the closely related radiative recombination rate. We give an especially simple but accurate approximation that works for any high hydrogenic level and can be conveniently employed in large-scale numerical simulations.

Subject headings: atomic data; atomic processes; diffuse matter

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1 Introduction

Plasma simulations are a powerful aid in the interpretation of astronomical spectra (Osterbrock 1989). However, the simulations must be as complete as possible to be valid. It is necessary to include all relevant physics, and large multi-level model atoms must often be incorporated. Today's fast computers make accomplishing this relatively routine.

We are a developing large spectral simulation code, Cloudy, which now includes an arbitrarily large multilevel model atom for all hydrogenic species (Ferland 2000). A complete simulation must include all processes that couple this atom to the surrounding gas. The atom interacts with its environment through the action of photoionization and photoelectric heating, and through radiative recombination and recombination cooling.

Although ab initio cross sections and rates could be computed on the fly, in practice these are pre-computed and fitted analytically. Examples include photoionization cross-sections or recombination rate coefficients, which we fit as described in Verner and Ferland (1996).

Currently, there are no state-specific hydrogenic recombination cooling rates, or analytical fits of these, for a wide range of energy levels and temperature. Ferland et al. (1992) and Hummer (1994) calculated recombination-cooling rates, and these are in excellent agreement, but the tabulated data and fits presented do not extend to higher levels, or include the range of temperature needed for highly charge species at nebular temperatures. This compromises modern simulations of emitting environments since there is no clear way to include cooling from these species.

In the following we present new calculations of the recombination cooling rates and make simple analytical fits that are valid for any quantum number n and for the temperature range of interest for thermal gas. These fits should allow this process to be included for any level, charge state, and temperature where it will be significant.

2 Calculations

Here we compute recombination and cooling rates for any level within a hydrogenic ion of charge Z. In the following the electron temperature is T, the energy level is n, the photoionization cross section is $a(Z, \varepsilon)$, and the photoelectron electron residual kinetic energy ($h\nu$-Z^2/n^2 in Ryd) is ε. The rate per unit volume at which ions recombine to the level n is $n_e\, n_p\, \alpha_n$ [cm^{-3} s^{-1}] where α_n is the radiative recombination rate coefficient for that level. This is given by (Seaton 1959, 1960; Brown & Mathews 1970; Gould 1971)

$$\alpha_n(T,Z) = \frac{c\alpha^3}{\sqrt{\pi}} Z^3 \lambda^{\frac{3}{2}} n^{-2} \int_0^\infty d\varepsilon\, (1+n^2\varepsilon)^2 e^{-\lambda\varepsilon} \widetilde{a}_n(Z,\varepsilon) \ \ [\mathrm{cm^3\ s^{-1}}]. \quad (1)$$

The corresponding cooling per unit volume for recombination to level n is given by $kT\beta_n$ [erg cm^{-3} s^{-1}] where β_n is the recombination-cooling coefficient given by

$$\beta_n(T,Z) = \frac{c\alpha^3}{\sqrt{\pi}} Z^3 \lambda^{\frac{5}{2}} n^{-2} \int_0^\infty d\varepsilon\, \varepsilon(1+n^2\varepsilon)^2 e^{-\lambda\varepsilon} \widetilde{a}_n(Z,\varepsilon)\, [\mathrm{cm^3\ s^{-1}}] \quad (2)$$

where

$$\frac{c\alpha^3}{\sqrt{\pi}} = 6572.6617 \ \ [\mathrm{cm\ s^{-1}}] \quad (3)$$

and

$$\lambda = \frac{Z^2}{T} 1.5789 \times 10^5. \quad (4)$$

The forms of equations 1 and 2 are similar enough that there should be a fairly simple relationship between the resulting quantities. If so, then once the ratio of the coefficients is known it becomes an easy task to establish both rates in terms of a single fitting formula.

We computed the recombination and cooling coefficients numerically for n between 1 and 400 and temperatures T between 10^3 and 10^{11} K. The numerical procedure was adjusted for different energy levels to maintain the same precision for all n.

Two different routines were used to determine the photoionization cross sections for various n and photon energy. For $n < 30$, nearly exact cross sections using routines created as part of the Opacity Project were used. For levels above 30 the simpler routine given by Verner & Ferland (1996) was used. Note that in this approach no gaunt factors are used, rather actual photoionization cross-sections are employed. For levels below 30 an accuracy well under 1% is expected, while for higher levels the overall accuracy is roughly 2 percent, limited by the accuracy of the second routine's fit of the photoionization cross sections. The results agreed with those presented by Ferland et al. (1992) and Hummer (1994) to much better than 1% for the levels where comparison was possible.

Figure 1 shows the computed results for the recombination and cooling rate coefficients. In this and later figures energy is shown as the charge-scaled energy T/Z^2. Overall the two figures appear quite similar, suggesting that a simple relationship holds between the two quantities. Figure 2 shows the ratio of cooling to recombination rate coefficient, $\gamma = \beta/\alpha$, as a function of n and T/Z^2. The ratio changes by about 1 dex, while α and β change by roughly 16 dex. Figure 3 shows the same plot, but uses a temperature scaled to the level's ionization potential, $t = Tn^2/Z^2$, as the independent axis.

Figure 3 shows that γ is nearly independent of n, except for the corner representing high t and low n. For the regions where results are nearly n-independent, the recombining electrons have an energy close to the photoionization threshold of the level. In terms of the photoionization cross section and the Milne relation, these recombinations occur on the power-law, near threshold, part of the photoionization cross section. In this case the temperature-weighted integral over cross section (equation 2) is independent of n except for a scale factor representing the photoionization cross section at threshold. This scale factor appears in both α and β and so cancels out in the ratio. This cancellation does not occur in the lower right corner, which represents the very highest temperatures. Here recombinations occur so far from threshold that non-power-law deviations in the photoionization cross-section become important. The effect is real, but only occurs at the highest temperatures.

The line in Figure 3 represents $T = 10^6$ K. For temperatures greater than this (regions to the lower right in the figure) bremsstrahlung will be far more important than free-bound cooling. For these temperatures recombination cooling can be treated with far less precision since it is negligible. If this region is excluded then the functional fit to γ is just a function of t and is independent of n.

Figure 4 shows γ for the particular case of n=150 and Table 1 gives some values. The function approaches an asymptote of 1 as $t \to 0$. This was found by analytically approximating the ratio at low t.

We fitted γ by piecewise continuous functions with the following form:

$$\gamma(t) = \frac{\beta_n(T_e, Z)}{\alpha_n(T_e, Z)}$$
$$= \left\{ \begin{array}{cc} 1 & t < 10^2 \\ a + bt + ct^{1.5} + dt^2 + et^2 \ln t & 10^2 \le t < 7.4\times10^5 \\ f + gt + h(\ln t)^2 + i/t^{0.5} + j\ln t/t^2 & 7.4\times10^5 \le t < 5\times10^{10} \\ \left(k + lt^{0.5} + m\ln t\right)^{-1} & 5\times10^{10} \le t < 3\times10^{14} \\ 1.289\times10^{11} t^{-0.9705} & 3\times10^{14} \le t \end{array} \right\} \quad (5)$$

where the coefficients are given in Table 2. This fit has an accuracy much greater than 1%.

3 An application

The expansion given above has been incorporated into the spectral simulation code Cloudy, last described by Ferland (2000). Previously the state-specific recombination-cooling coefficients for the lowest 6 levels of hydrogen were taken from Ferland et al. (1992) and for higher levels rough scale factors were derived from examination of the more extensive tables of Hummer (1994).

The current implementation combines equation 5 with the extensive fits to radiative recombination rates given by the routine **`hrfit`**, presented in Verner & Ferland (1996) and available on the web at http://www.pa.uky.edu/~verner/atom.html . That routine evaluates radiative recombination rate coefficients for $n < 400$ and temperatures below 10^9 K. The free-bound cooling is evaluated by combining those results with the calculations presented here.

To cite one extreme example, the quasar Broad Emission Line Region calculation presented in Ferland et al. (1992) was recomputed with a large hydrogen atom (50 levels) and the cooling rates given here. The lower half dozen levels of hydrogen are optically thick in this model and a substantial part of the cooling is carried by higher recombinations. The improved treatment described here increases the recombination cooling by roughly 20%. The differences are smaller in less extreme models.

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5 Figures

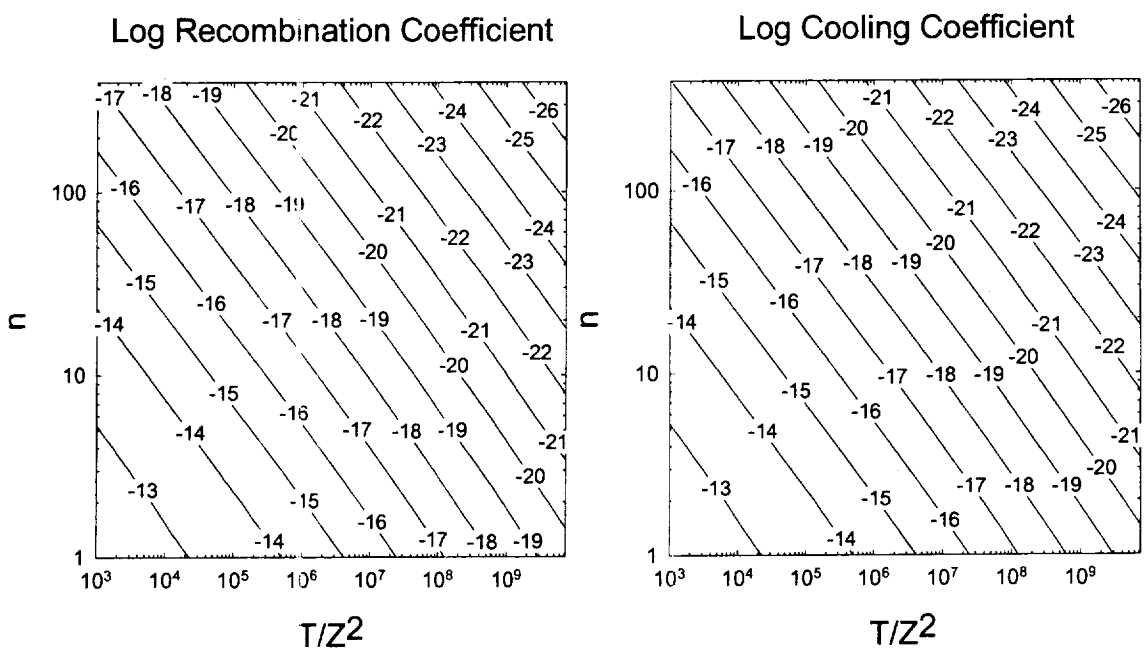

Fig. 1 – Recombination and cooling coefficients. These are show for various quantum numbers (the vertical axis) and charge-scaled temperatures (the horizontal axis). These each vary by 13 orders of magnitude over the plotted range.

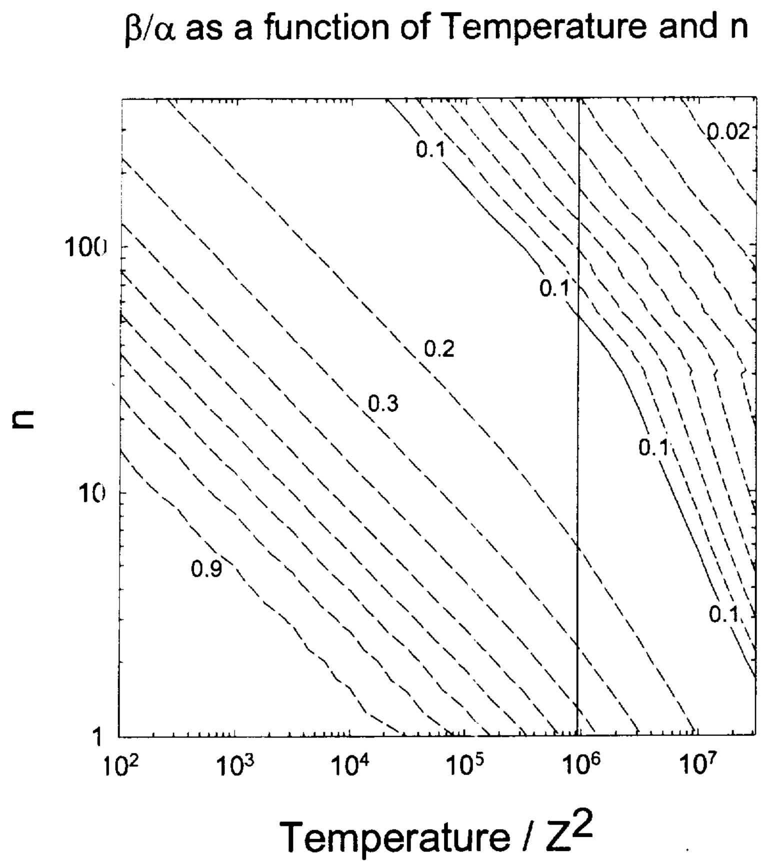

Fig. 2 – Ratio of the cooling coefficient to the radiative recombination rate coefficient. The quantum number is shown as the vertical axis, and the charge-scaled temperature is the horizontal axis. Although the cooling and recombination coefficients each vary by 13 orders of magnitude over the plotted range, their ratio varies by less than one hundred.

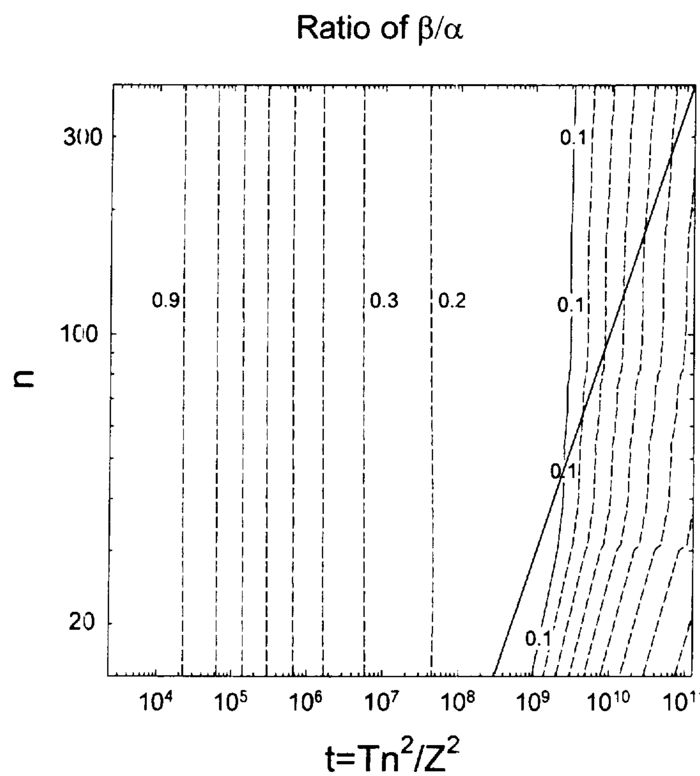

Fig. 3 – Ratio of cooling to recombination, with Tn^2/Z^2 as the independent axis. By rescaling the temperature to become the temperature relative to the ionization potential the dependence on quantum number is nearly removed. Regions to the lower right of the slanting line are too hot for recombination cooling to compete with the dominant bremsstrahlung cooling, and are not fitted in this work.

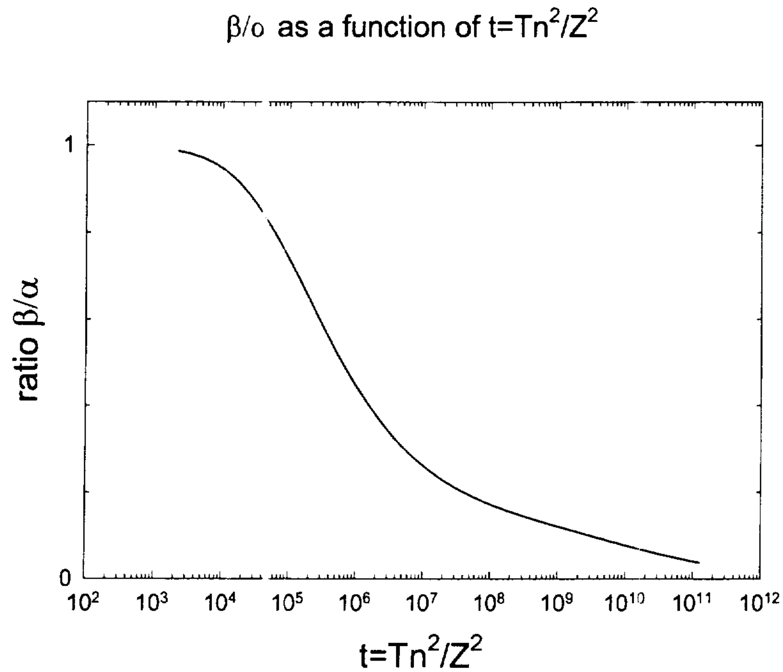

Fig 4 – The ratio β/α vs Tn^2/Z^2. For regions to the left of the line in Figure 3 the results are only a function of the scaled temperature t. This figure plots this function, which is fitted by equation 5.

6 Tables

Table 1 Values of γ for n=150 and selected $t=Tn^2/Z^2$

t	γ	t	γ	t	γ	t	γ
6.57E+01	0.999596	2.49E+06	0.357823	9.42E+10	0.0411226	5.35E+15	9.11E-05
1.48E+02	0.999075	5.60E+06	0.296685	2.12E+11	0.0311245	1.20E+16	4.11E-05
3.33E+02	0.997925	1.26E+07	0.249445	4.77E+11	0.0230145	2.71E+16	1.84E-05
7.48E+02	0.995368	2.83E+07	0.213222	1.07E+12	0.0166741	6.10E+16	8.19E-06
1.68E+03	0.989754	6.38E+07	0.185226	2.42E+12	0.0118725	1.37E+17	3.64E-06
3.79E+03	0.97777	1.43E+08	0.162949	5.43E+12	0.0083326	3.09E+17	1.62E-06
8.52E+03	0.95356	3.23E+08	0.144256	1.22E+13	0.00577985	6.95E+17	7.20E-07
1.92E+04	0.909123	7.26E+08	0.127504	2.75E+13	0.00397167	1.56E+18	3.20E-07
4.31E+04	0.838294	1.63E+09	0.111615	6.19E+13	0.00270783	3.52E+18	1.42E-07
9.71E+04	0.743103	3.68E+09	0.0960789	1.39E+14	0.00180685	7.91E+18	6.32E-08
2.18E+05	0.635148	8.27E+09	0.0808811	3.13E+14	0.00110269	1.78E+19	2.81E-08
4.91E+05	0.529034	1.86E+10	0.0663478	7.05E+14	0.000592699	4.01E+19	1.25E-08
1.11E+06	0.435189	4.19E+10	0.0529515	1.59E+15	0.000290197	9.01E+19	5.55E-09

Table 2 Fitting coefficients for γ in equation 5

a	1.00028519708435	f	0.2731170438382388	k	-17.028197093979
b	-7.569939287228937E-06	g	6.086879204730784E-14	l	4.516090033327356E-05
c	2.791888868562404E-08	h	-0.0003748988159766978	m	1.08832467825823
d	-1.289820289839189E-10	i	270.245476366191		
e	7.829204293134294E-12	j	-1982634355.34978		